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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
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10/530,550

04/07/2005

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EXAMINER

BORIN, MICHAEL L

ART UNIT

PAPER NUMBER

1631

MAIL DATE

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PAPER

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

<b>Office Action Summary</b>	<b>Application No.</b> 10/530,550	<b>Applicant(s)</b> KOTANI ET AL.	
	<b>Examiner</b> Michael Borin	<b>Art Unit</b> 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

### Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

### Status

- 1) ☒ Responsive to communication(s) filed on 11 July 2008.
- 2a) ☒ This action is **FINAL**.                      2b) ☐ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

### Disposition of Claims

- 4) ☒ Claim(s) 1,4,7 and 8 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☒ Claim(s) 1,4,7 and 8 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

### Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on \_\_\_\_\_ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.  
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

### Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All    b) ☐ Some \*    c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
  2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
  3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

\* See the attached detailed Office action for a list of the certified copies not received.

### Attachment(s)

- |  |   |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892)          | 4) <input type="checkbox"/> Interview Summary (PTO-413)           |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____                                      |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08)          | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date _____  | 6) <input type="checkbox"/> Other: _____                          |

## **DETAILED ACTION**

### **Status of Claims**

1. Amendment filed 07/11/2008 is acknowledged. Claims 2,3,5,6,are canceled.  
Claims 7,8 are added. Claims 1,4,7,8 are pending.

Claims 1,4 are amended. Amendments to the claims necessitated new grounds of indefiniteness rejections under 35 U.S.C. 112, second paragraph, and/or did not obviate the rejections under 35 U.S.C. 112, second paragraph, made in the previous Office action. Since the claims remain vague and indefinite, no art rejection was made in this Office action; however, some pertinent prior art is listed in "Prior Art of Record" section.

### ***Claim Rejections - 35 USC § 112, second paragraph.***

The following is a quotation of the second paragraph of 35 U.S.C. 112:

The specification shall conclude with one or more claims particularly pointing out and distinctly claiming the subject matter which the applicant regards as his invention.

2. Claims 1,4, 7,8 are rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

The reasons rejection is applied for the following reasons as applied to claim 1; consequently, claims 4, 7,8 are rejected for the same reasons.

Amendments to the claims necessitated the following new grounds of rejection:

H. Claim 1: The language of the preamble: "method for determining and displaying physicochemical characteristics of a compound ... which modulates pharmacological activity of the compound". It is not clear how an existing characteristics of a compound might modulate (in which way?) pharmacological activity of said compound.

In addition, the preamble addresses a plurality of physicochemical characteristics of a compound. At the same time, the preamble addresses a singular characteristic "which modulates". The language is confusing as it is not clear which one of the plurality of characteristics is being determined, displayed and is addressed as modulating pharmacological activity of the compound.

Please clarify via clearer claim language.

I. Claim 1, process A: It is unclear which "plurality of molecules" is being superposed. Do these molecules have any relationship to each other?

J. Claim 1, process C: the process is addressed as calculating interaction between atoms and "represented points". The latter, "represented points", is a calculated coordinates in virtual space. It is not clear how atoms may have "interaction" with such "represented points". In particular, it is not clear how an atom and a "represented point" may have such interactions as steric, electrostatic, or hydrophobic. Furthermore, even if the claims addressed interactions between atoms, it is not clear what kind of hydrophobic interactions is meant since atoms, unlike molecules, are not engaged in such types of interactions.

Note, that Fig. 3 to which applicant refers provides no clarification of the issue.

K. Claim 1, process D: process D is directed to correlating statistical analysis of interactions between atoms and “represented points”. As addressed in the preceding paragraph, it is not clear what is the significance of interaction between an atoms and an arbitrary “represented point”.

Further, it is not clear how and what plurality of “correlation coefficients” is being calculated, and what “activity predicting formula” is being formed.

L Claim 1, process E: process E is directed to assigning “activity predicting value” to an atom. First, it is not clear how such value is being generated – the specification does not address “activity predicting value” for atoms. Do atoms (as opposed to molecules) have pharmacological activity? Second, it is not clear how, having obtained [unidentified] correlation of interactions between atoms and “represented points with a pharmacological activity of one of molecules, an [unidentified] activity is assigned to each and every atom of each and every molecule.

M. Claim 1, steps C, B2: It is not clear whether atomic distances in step B2 are calculated for atoms of the same molecule or different molecules. Please clarify.

The following rejections under 35 U.S.C. 112, second paragraph, in the preceding Office action are being maintained.

A. Claim 1 is indefinite due to the lack of clarity of the claim language failing to recite a final process step, which agrees back with the preamble. The preamble states that it is a method of displaying characteristics of a compound that modulate pharmacological

activity of the compound, however the claim recites a final step of assigning activity prediction values to atoms, which is not indicative of characteristics that modulate pharmacological activity of the compound.

Fig. 1 and p. 30 to which applicant refers does not seem to clarify the issue.

F. Claim 1, step C. The meaning of calculating interactions between atoms and points is not clear. How atoms interact with points?

If the by points the pseudo-atoms are meant (which are being simply a set of coordinates), what kind of interaction of atoms with set of coordinates is meant?

And how such interactions are being “calculated”?

Furthermore, with respect to claim 3, how an interaction such as electrostatic or hydrophobic” can be calculated for interaction between an atom and a point or a set of coordinates?

Applicant points out that the claim as amended clarifies what interactions are meant. However, as addressed in the new rejection “J” above, this remains the most confusing issue. Applicant points out at the substantial portion of specification, p. 30, 34-67 as examples of “specific selections for the interactions”; however, said portion of specification does not seem to explain interaction between interactions between atoms and points as now claimed. Please clarify.

G. Claim 1, step D: Since the nature of “calculating interactions” is unclear, it is equally unclear how the interactions are being analyzed.

Applicant submits that amendment to the claim clarifies the issue. However, it remains unclear in Examiner's opinion – see new rejections “J” and “K” above.

Note that in view of the vagueness and indefiniteness of the claims, as addressed above, rejections over prior art are not being applied at this point.

***Claim Rejections - 35 USC § 112, first paragraph.***

The following is a quotation of the first paragraph of 35 U.S.C. 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

3. Claims 1,4,7,8 are rejected under 35 U.S.C. 112, first paragraph, as containing subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventors, at the time the application was filed, had possession of the claimed invention. The rejection is applied for the following reasons:

A. Claims 1,4 introduce new matter as they use the phrase “assigning activity prediction value to each atom”. There is no disclosure in the specification of “assigning activity prediction value to each atom” and there is no guidance on how to practice the claimed method as instantly claimed.

B. Claims 6,7 introduce new matter as address using “evaluation formulas” of “rapid molecular superstition”, and “indicated variables”. Such formulas for calculating

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interactions (which interactions?) of atoms and “represented points” are not described in the specification.

***Claim Rejections - 35 U.S.C. § 101/ 112-1***

The following is a quotation of the 35 U.S.C. § 101:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter or any new and useful improvement thereof, may obtain a patent therefore, subject to the conditions and requirements of this title.

The following is a quotation of the first paragraph of 35 U.S.C. § 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

4. Claims 1,4,7,8 are rejected under 35 U.S.C. § 101 because the claimed invention lacks patentable utility due to its not being supported by either specific and/or substantial utility or a well established utility.

Claims 1,3,4,6 are rejected under 35 U.S.C. § 101 because the claimed invention is not supported by either a specific and substantial asserted utility or a well established utility. The claims are drawn to a method for determining and displaying physicochemical characteristics of a compound ... which modulates pharmacological activity of the compound”. As it is not clear how an existing characteristics of a compound might modulate (in unidentified way) a pharmacological activity of said



compound, and it is not clear how an “activity prediction value to each atom” in multiple molecules allows determining and displaying physicochemical characteristics of compound ... which modulates pharmacological activity of the compound, neither substantial nor specific utility appears to be provided for the invention as claimed. At best, the invention as claimed is an invitation for a basic research.

The rejection is revised to address amendments to the claims.

Applicant refers to Fig. 3 which, however, is not viewed as supporting a specific or substantial utility of the method as claimed. Applicant further argues that the claims recite a method for “determining and visually displaying physicochemical properties of a compound”. The claims, however, are directed to displaying “activity prediction value” related to each atom. As atoms, unlike molecules, do not have “activity”, this is not viewed as a “real world” practical result. As it is not clear how an existing characteristics of a compound might modulate (in unidentified way) a pharmacological activity of said compound, and it is not clear how an “activity prediction value to each atom” in multiple molecules allows determining and displaying physicochemical characteristics of compound ... which modulates pharmacological activity of the compound, neither substantial nor specific utility appears to be provided for the invention as claimed. At best, the invention as claimed is an invitation for a basic research.

5. Claims 1,4,7,8 are also rejected under 35 U.S.C. §112, first paragraph. Specifically, since the claimed invention is not supported by either a credible asserted utility or a well established utility, one skilled in the art would not know how to use the claimed invention.

***Claim Rejections - 35 U.S.C. § 101(non-statutory invention)***

The following is a quotation of the 35 U.S.C. § 101:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter or any new and useful improvement thereof, may obtain a patent therefore, subject to the conditions and requirements of this title.

6. Claims 1,4,6,7 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

The claims are directed to a computational method.

To qualify as a statutory process, the claims should positively recite the other statutory class (the thing or product) to which it is tied, for example by identifying the apparatus that accomplishes the method steps, or positively recite the subject matter that is being transformed, for example by identifying the material that is being changed to a different state or thing. Nominal data gathering or post solution activity steps in the claimed subject matter will not be considered sufficient to convert a process that otherwise recites only mental steps into statutory subject matter. Steps directed to pre- or post-solution activity, or preamble limitations that require the claimed process to comprise machine implemented steps, will not be considered sufficient to convert a process that otherwise recites only mental steps into statutory subject matter. The applicants are cautioned against introduction of new matter in an amendment.

Further, the claims do not satisfy "useful, tangible, and concrete" requirements for the inventions directed to a 35 U.S.C 101 judicial exception.

First, the instant claims do not satisfy the "useful" prong of requirement for claims directed to judicial exceptions. For an invention to be "useful" it must satisfy the utility requirement of section 101, i.e., it has to be (i) specific, (ii) substantial and (iii) credible. As discussed in the utility rejection above, the invention does not satisfy the criteria of utility requirements as not being specific and substantial. Furthermore, claims must be limited only to statutory embodiments. The instant claims seem to be directed to calculation of an abstract interactions between points in the space with atoms of molecules. Such calculation results in an "activity prediction value" related to each atom. As atoms, unlike molecules, do not have "activity", this is not viewed as a "real world" practical result.

Second, the claims do not satisfy the "concrete" prong of requirement for claims directed to judicial exceptions, as it does not seem to be producing the same result if repeated by another person.

The method is directed to analysis of interaction of atoms of molecules superposed in virtual space. As discussed in the specification, p. 2, last paragraph

The approach of superposing atoms with each other has a disadvantage that researcher's subject is inevitably reflected, and ... subjective superposition of different molecules one atop the other by a researcher may result in something which is quite different from superposition of conformations in which actual molecules interact

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Even though the cited section of specification addresses prior art in background information, the claimed method is directed to post-superposition steps (see p. 3, line 16), therefore, the issues addressed above remain. Thus, the method comprises a step of “subjective superposition of different molecules one atop the other by a researcher”, which will result in a method which is not “concrete”.

Taken together, the claims are directed to non-statutory subject matter as the claimed invention does not “transform” an article or physical object to a different state or thing and the final result achieved by the claimed invention does not satisfy the criteria of being useful, and concrete.

Furthermore, in regard to claims 4,7 “Computer-Related Inventions” section of the MPEP at section 2106, Part IV, subpart B, also clarifies that claiming non-statutory subject matter on a computer medium or in software does not prevent this rejection. Claims 4,7 are directed to a program which is not a statutory subject matter. Computer programs do not define any structural and functional interrelationships between the computer program and other claimed elements of a computer which permit the computer program's functionality to be realized

## **Response to arguments**

With respect to “useful” result, applicant argues that the method “reduces computing resources”. The alleged reduction of the resources however does not produce a result which can be viewed as real world practical result. Further, applicant argues that the method provides detailed information about atom interactions that permits synthesizing molecules with enhanced activity. There is no nexus, however, between the determined “activity prediction value” for atoms with characteristics which modulate activity of a compound, and further, with synthesizing molecules with enhanced activity.

With respect to “tangible” result, Examiner acknowledges that the added step of “displaying the activity prediction value ” satisfies the requirement.

With respect to “concrete” result, applicant argues that researcher’s subjectiveness addressed in the rejection is “ameliorated by cluster analysis and evaluation functions employed in the method.” Examiner disagrees. There are no “evaluation functions” addressed in the claims and the cluster analysis is viewed as the claimed method is directed to post-superposition steps (see p. 3, line 16), therefore, the issues addressed above remain.

***Prior art made of record***

7. The prior art made of record and not relied upon is considered pertinent to applicant’s disclosure:

- Cramer et al. (US 5,025,388);

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- Belvisi et al. Journal of Computer-Aided Molecular Design, 8 (1994) 211-220;
- Matter, H. J. Med. Chem. 1997, 40, 1219-1229;
- Lin et al. J. Chem. Inf. Comput. Sci. 2002, 42, 1490-1504

***Conclusion.***

8. No claims are allowed

9. Applicant's amendment necessitated the new ground(s) of rejection presented in this Office action. Accordingly, **THIS ACTION IS MADE FINAL**. See MPEP § 706.07(a). Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE MONTHS from the mailing date of this action. In the event a first reply is filed within TWO MONTHS of the mailing date of this final action and the advisory action is not mailed until after the end of the THREE-MONTH shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than SIX MONTHS from the date of this final action.

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Any inquiry concerning this communication or earlier communications from the examiner should be directed to Michael Borin whose telephone number is (571) 272-0713. The examiner can normally be reached on 9am-5pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran can be reached on (571) 272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/Michael Borin, Ph.D./  
Primary Examiner, Art Unit 1631

mlb